Organic jan 17

Tuesday, January 17, 2023 4:20 PM

Q. Relative Contribution order of Resonating Strs in Resonance hybrid formation?

i) $CH_2=CH-\overset{+}{C}H-\overset{-}{C}H-CH=CH_2$

ii) $CH_2=CH-\overset{\oplus}{C}H-CH=CH-\overset{\ominus}{C}H_2$ cross conj

iii) $\overset{\oplus}{C}H_2-CH=CH-CH=CH-\overset{\ominus}{C}H_2$ Extended conj

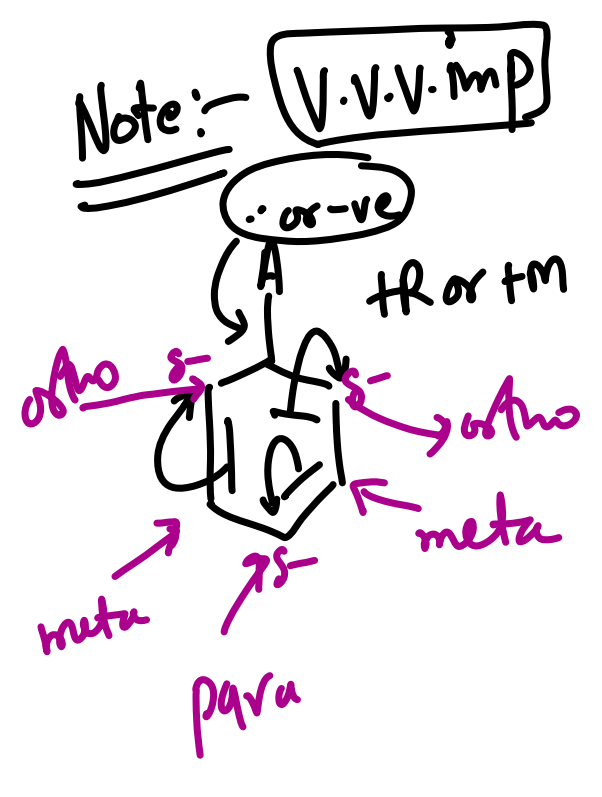
$\boxed{(i) > (iii) > (ii)}$

(**) Charge separatⁿ ↑es, Stability ↓es
distance b/w +ve & -ve

→ Provided Extended Conjugatⁿ is not present.

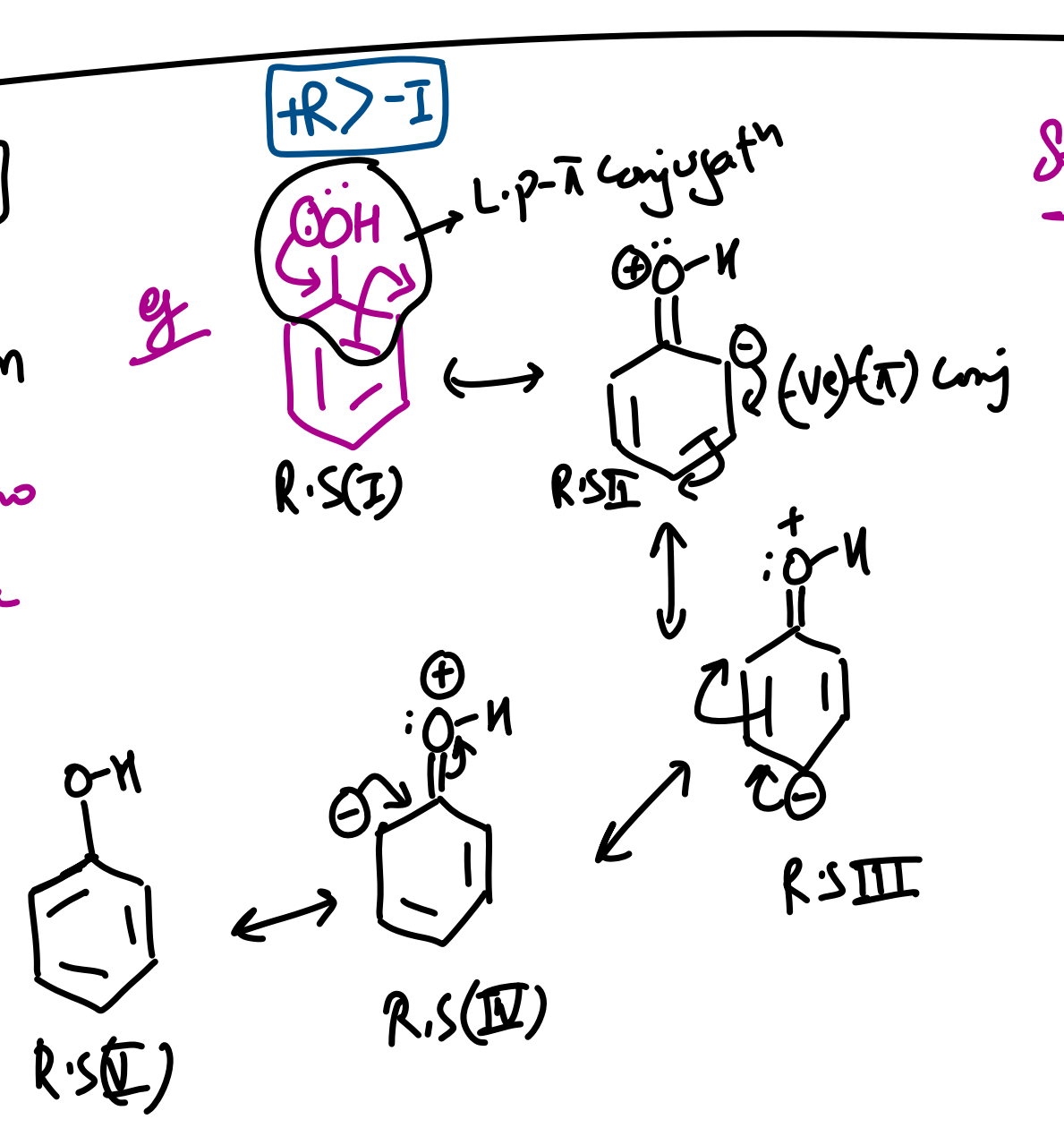
If extended conj is present, then Ext. conjugatⁿ dominates over charge separatⁿ.

Note:- V.V.V.imp



+R > -I

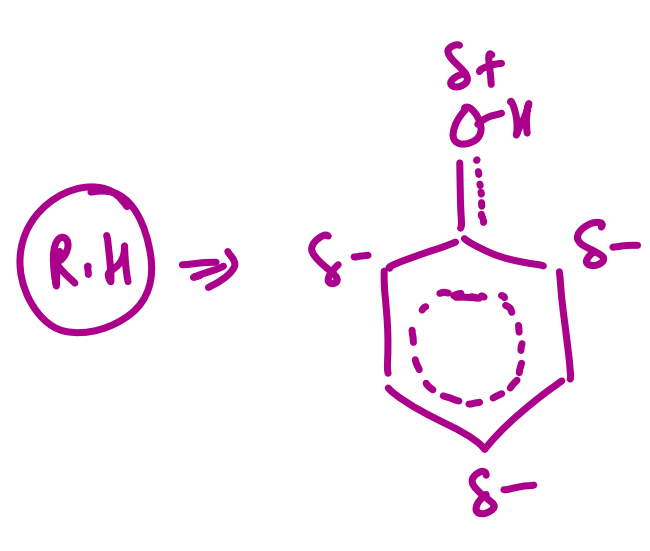
e.g.



Stability

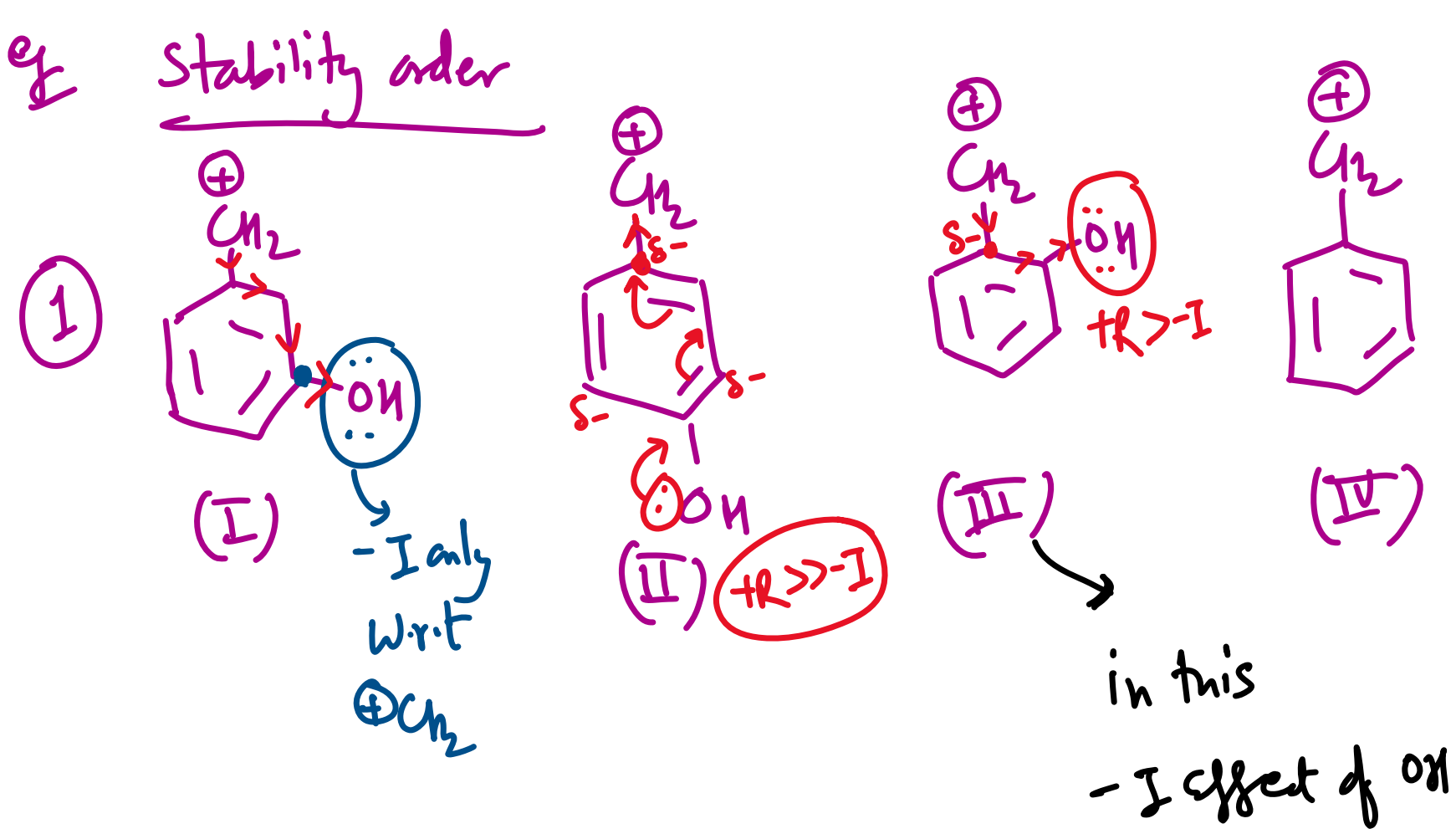
RS V = RS I > R.S II = RS IV > RS III

(R.H) ⇒



e.g. Stability order

(1)



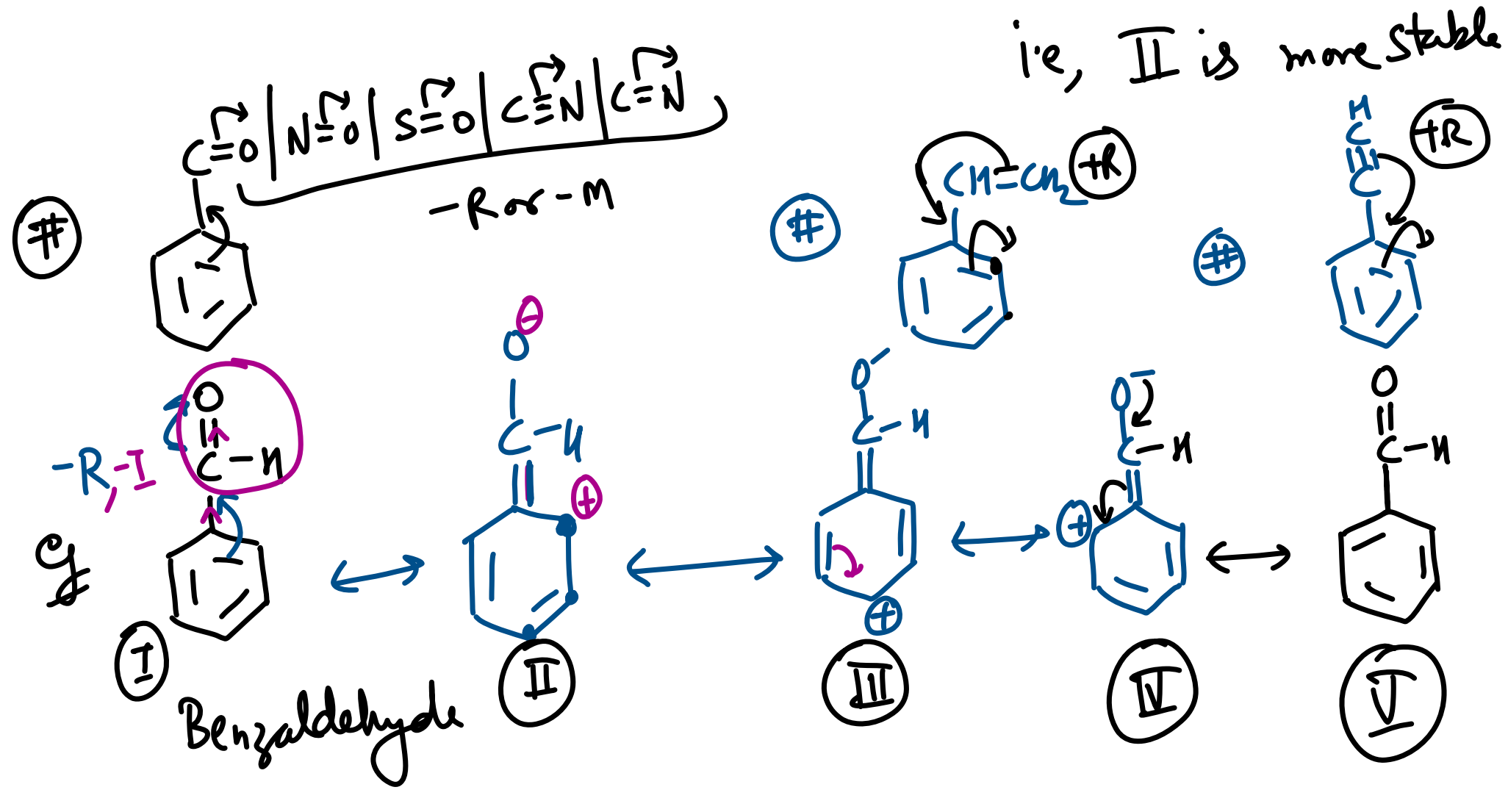
-I only w.r.t. ⊕CH₂

(II) +R >> -I

II > III > IV > (I)

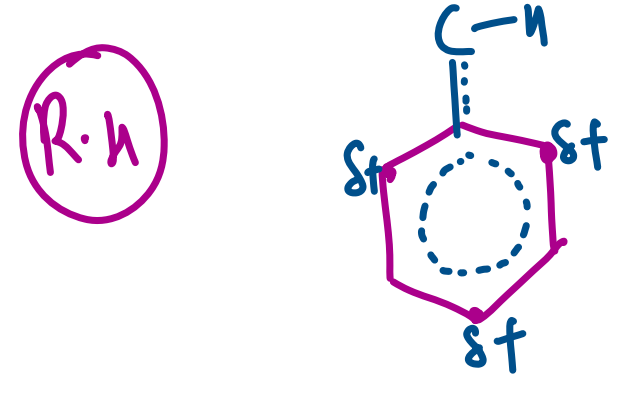
(III) → in this -I effect of OH is more than in (II) towards ⊕CH₂ i.e, II is more stable.

(**) Resonance is distance independent or M-effect
But Inductive effect is distance dependent.



Stability I = V > II = IV > III

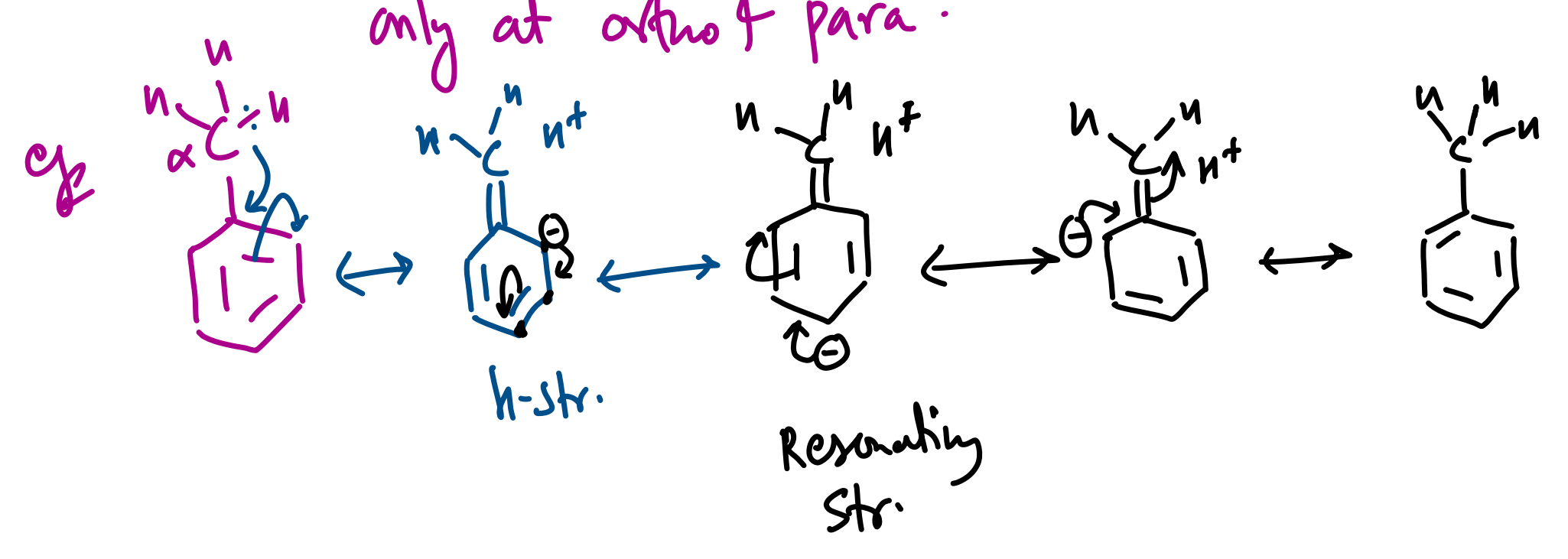
(R.H)



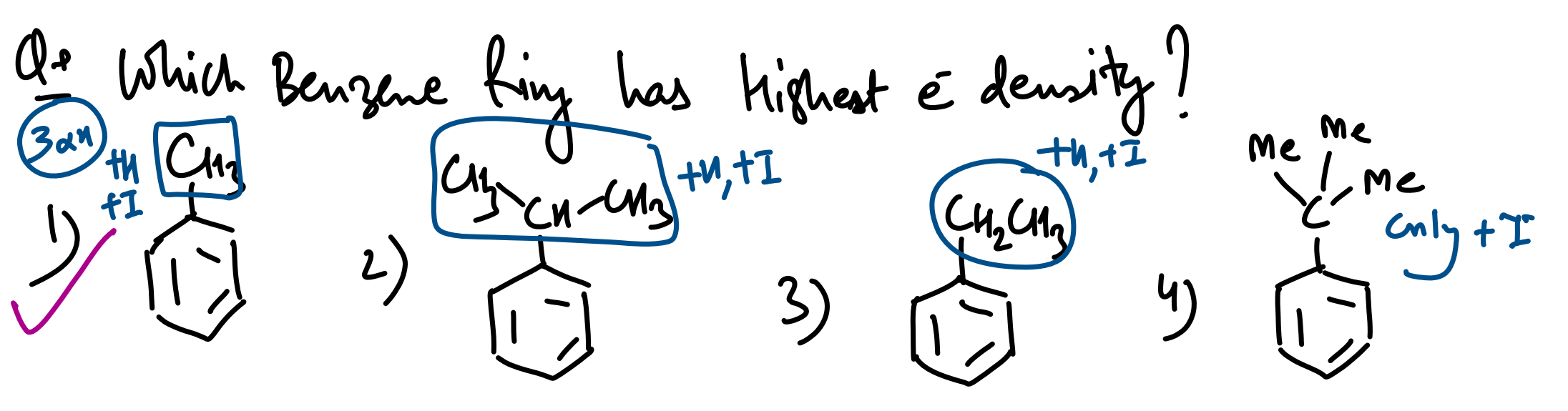
⇒ +R or -R always affect group present at ortho & para & doesn't affect group at meta position.

Similarly (+H) effect ↑es e⁻ density only at ortho & para.

e.g.



Q. Which Benzene Ring has Highest e⁻ density?



+H effect order ⇒ $-CH_3 > -CH_2-CH_3 > -CH(CH_3)_2 > -C(CH_3)_3$

+I effect ⇒ $-CH_3 < -CH_2-CH_3 < -CH(CH_3)_2 < -C(CH_3)_3$

→ +H effect dominates over +I

So, CH₃ is best EDG.

Aromaticity

Aromatic (Aro)

- → Cyclic
- → planar (All atoms present in Ring must be in same plane) i.e; all atoms are sp/sp² Hybridised
- → π e⁻ delocalisatⁿ (or Resonance) must occur in complete Ring & follow $(4n+2)\pi e^-$

n=0, 2πe⁻
n=1, 6πe⁻
n=2, 10πe⁻
n=3, 14πe⁻
n=4, 18πe⁻
n=5, 22πe⁻
⋮

HUCKEL'S RULE

(AA) Anti-Aromatic

Cyclic
planar (same)
→ π e⁻ delocalisatⁿ in complete Ring & involve 4nπe⁻

n=1, 4πe⁻
n=2, 8πe⁻
n=3, 12πe⁻
n=4, 16πe⁻
⋮

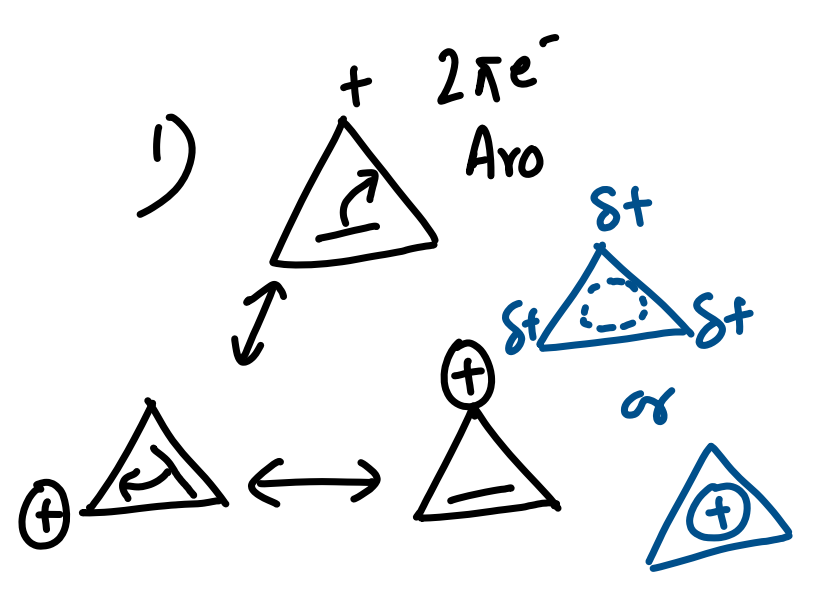
(NA) Non-Aromatic

Cyclic
π e⁻ delocalisatⁿ does not occur in complete ring Because either all Ring atoms not in one plane or atleast one carbon of Ring is sp³.

Stability:- Aro > NA >> (A.A) → least stable because Anti-Bonding molecular orbitals are involved for π e⁻ delocalisatⁿ.

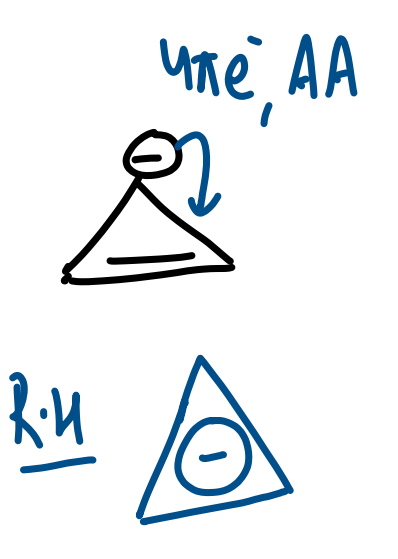
Q Identify Aro, Anti-Aro, Non-Aromatic?

1)



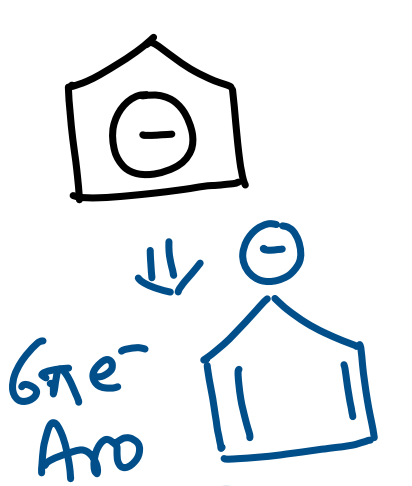
2πe⁻ Aro

2)



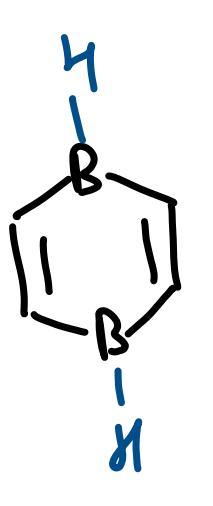
4πe⁻, AA

3)



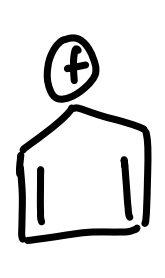
6πe⁻ Aro

4)



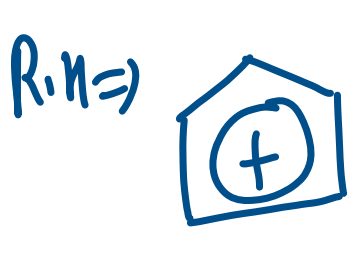
4πe⁻ A.A

5)

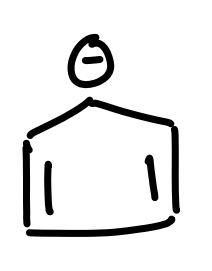


4πe⁻ A.A

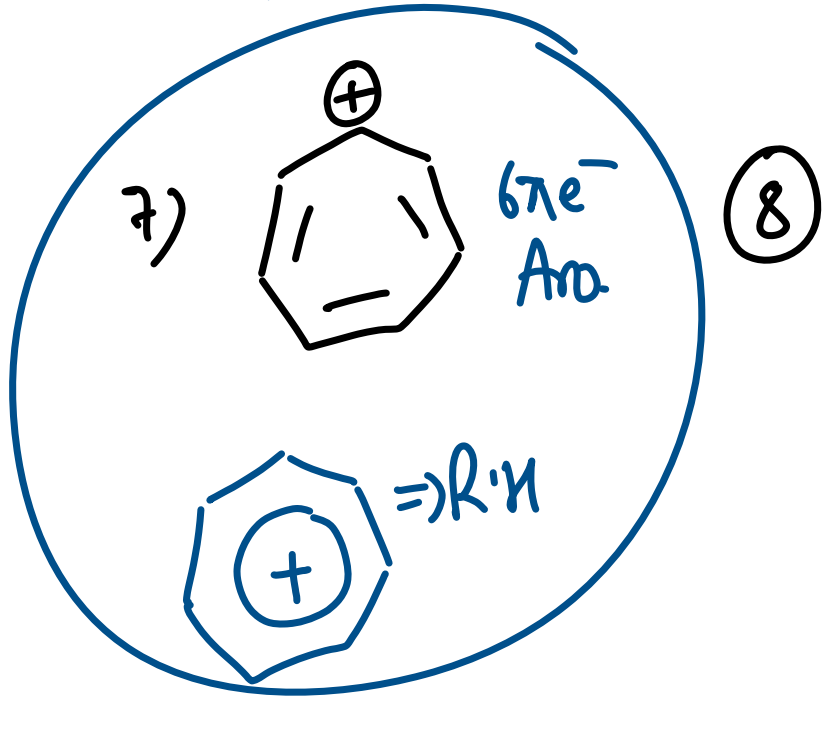
R.H ⇒



6)

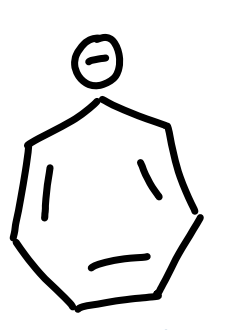


Aro



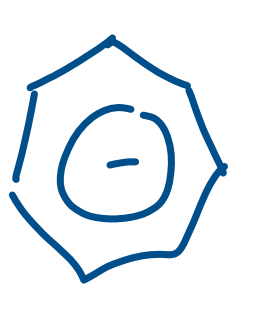
6πe⁻ Aro

(8)

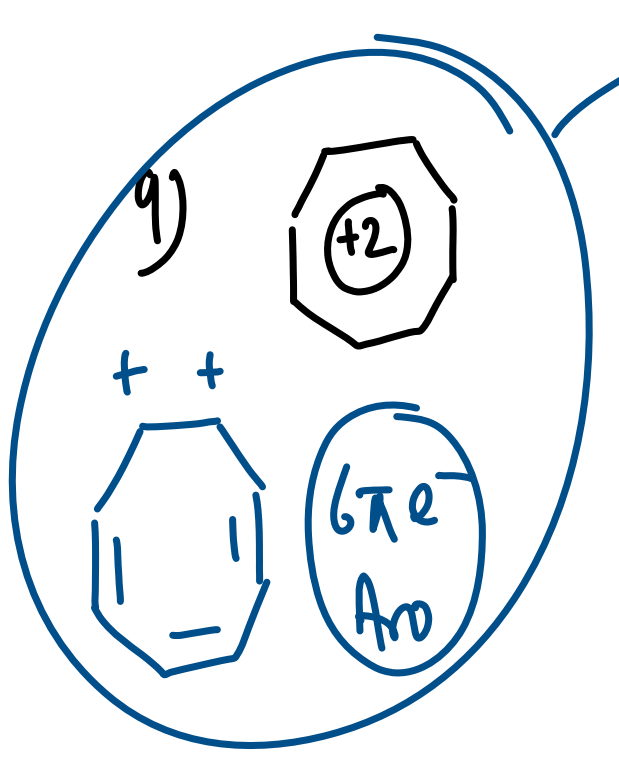


8πe⁻ A.A

R.H ⇒

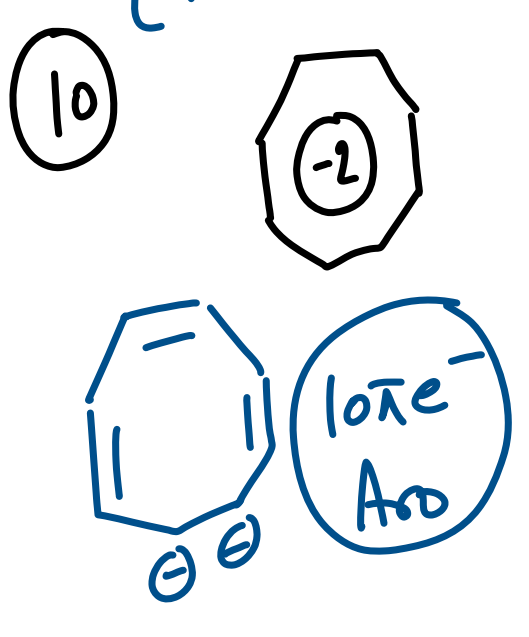


7 > 9 (stable)



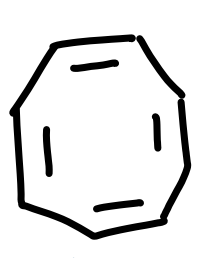
6πe⁻ Aro

(10)



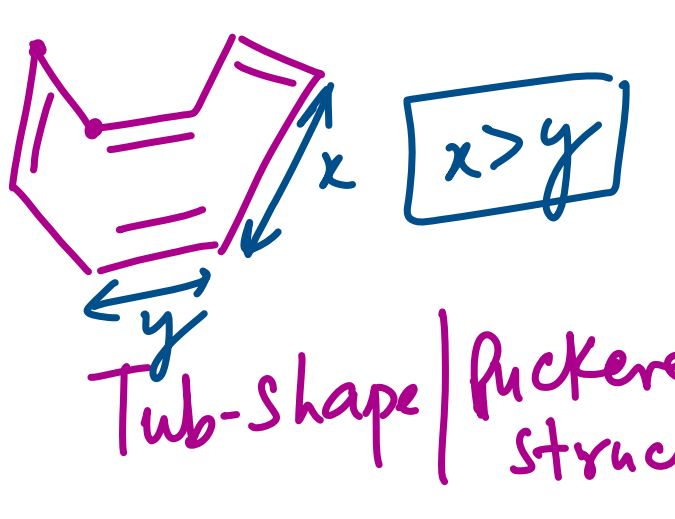
10πe⁻ Aro

(11)



C_8H_8

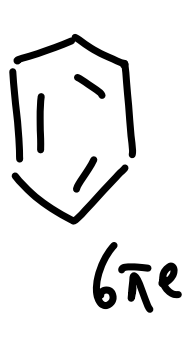
8πe⁻ ↳ shud be A.A, But it is non-Aromatic due to non-planar structure



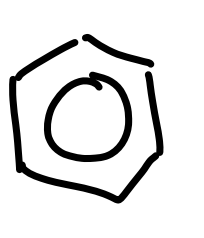
Tub-shape | Puckered structure

No Resonance → So different Bond lengths observed

12)

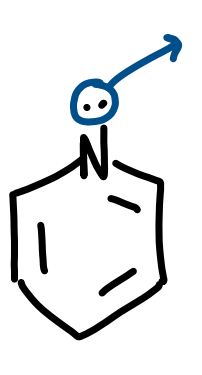


6πe⁻



all C-C Bonds are equal & have partial double Bond Character

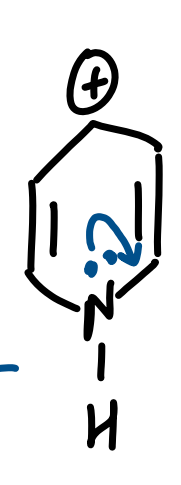
13



localised

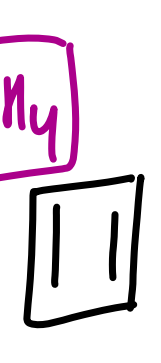
6πe⁻ Aromatic

14)



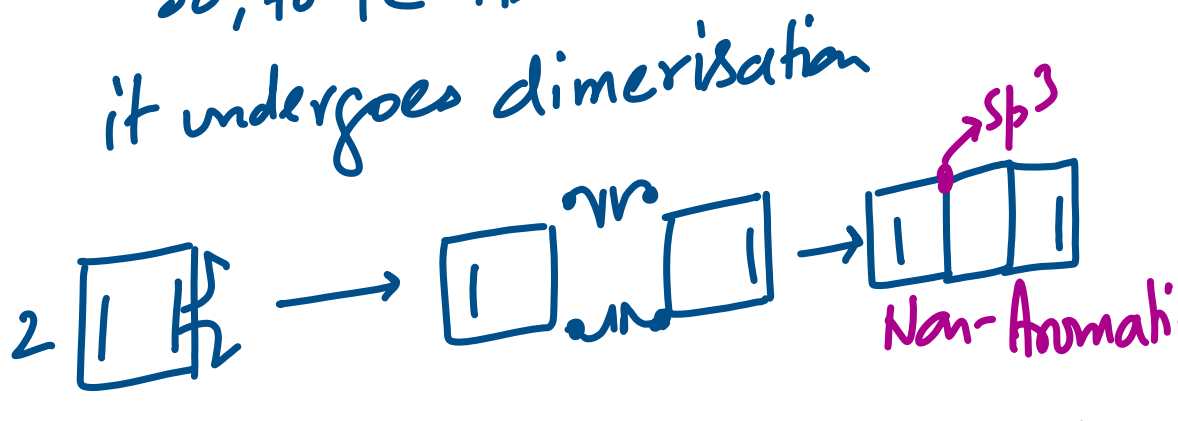
6πe⁻ Aro

15) C_4H_4



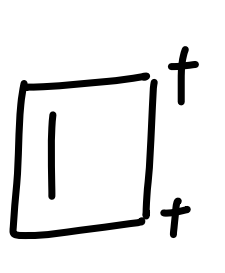
4πe⁻ A.A

So, to ↑e its stability it undergoes dimerisation



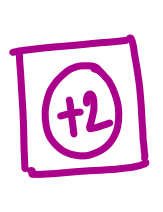
Non-Aromatic

16)

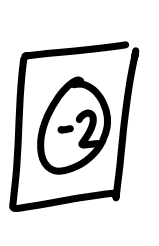


2πe⁻ Aro

R.H ⇒

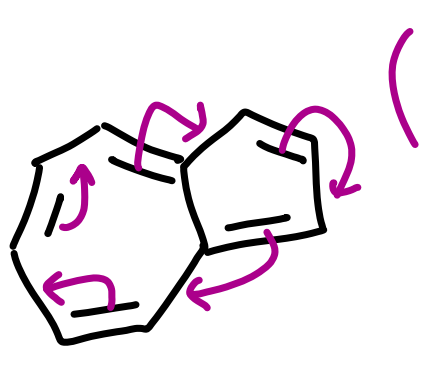


17)



6πe⁻ Aro

18)



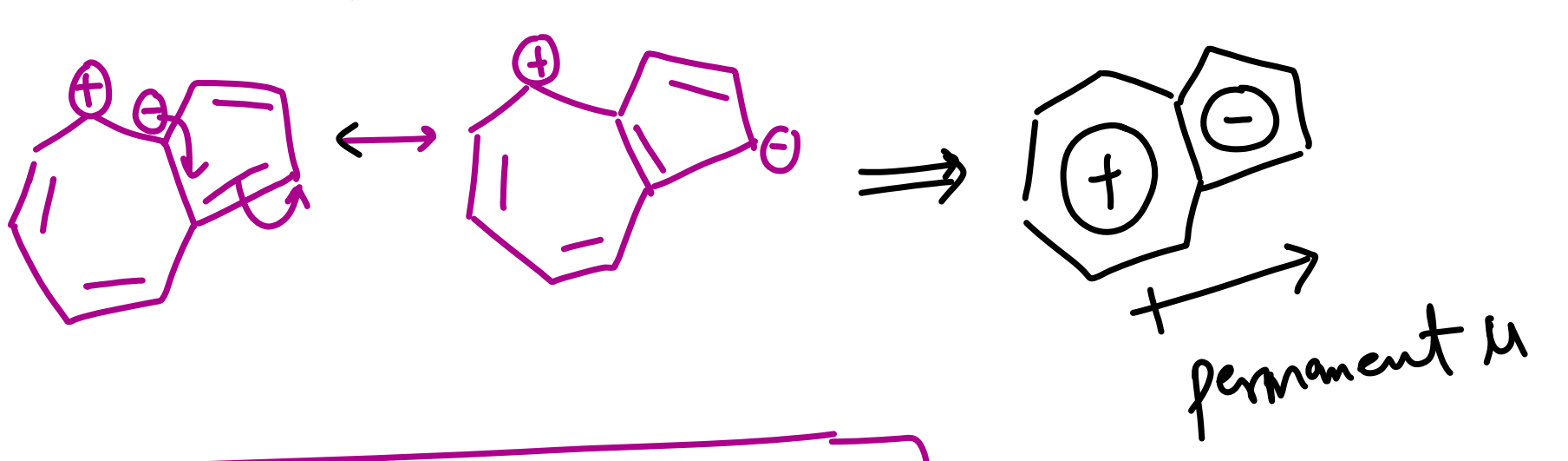
(fused Ring System) → only surface πe⁻s are counted

Azulene

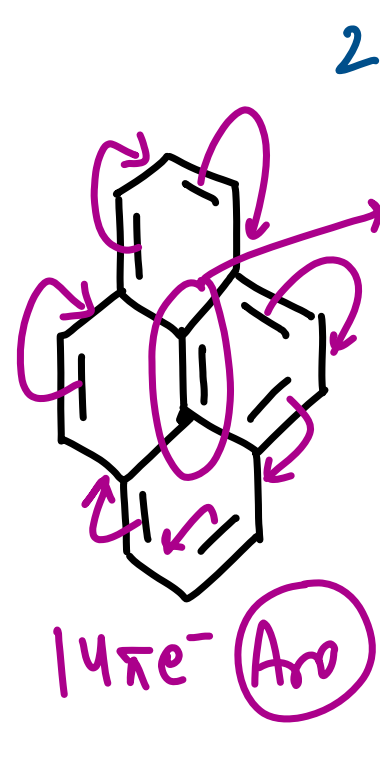
10πe⁻ (Aro)

→ This is dark colored.

→ have permanent dipole moment



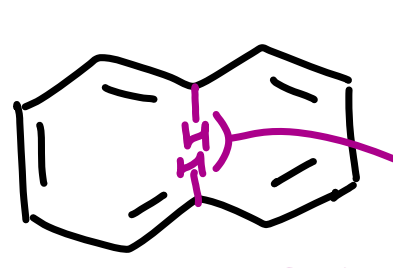
19)



not considered

14πe⁻ (Aro)

20)

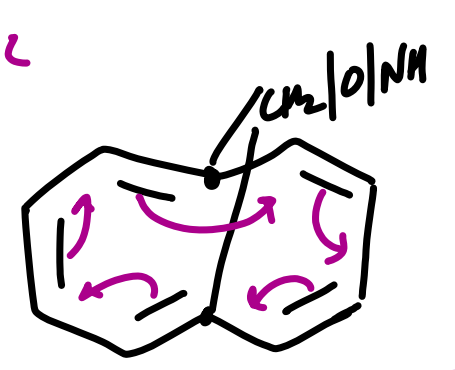


flagpole Replⁿ

$C_{10}H_{10} \Rightarrow [10]$-Annulene

Shud be Aro, But is non-Aromatic due to non-planar str.

21)



Aromatic

22) $C_{20}H_{20}^{2-}$

22πe⁻ Aro

23) [6]-Annulene

Aro

24) $C_4H_4^{2+}$

2πe⁻ Aro

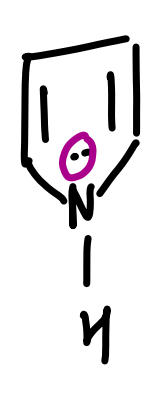
[n]-Annulene

Note:- $C_nH_n \Rightarrow$ Conjugated Cyclic Comp.

no. of C = no. of H = no. of πe⁻

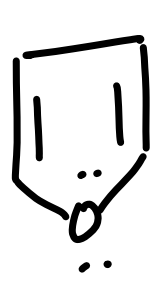
$C_4H_4^{2+} \Rightarrow 2\pi e^-$ (Aro)

25)



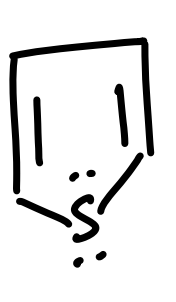
Aro

26)



Aro

27)



Aro